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Reconstruction of thermo-physical properties to improve material database for casting simulation

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Abstract. In this work, an advanced method is proposed for computational recovery of thermo-physical properties in a wide range from room temperature to values above the alloy melting point. This method allows us to improve material databases of CAE (Computer-Aided Engineering) programs for simulation of high-temperature technological processes. In most cases, computation of unsteady temperature fields is an important stage of CAE analysis in mechanical engineering. Moreover, various manufacturing technologies such as casting, welding, surface hardening, coating, heat treatment provide the desired material structure and its strength by controlling temperature field during solidification and subsequent cooling of a machine part. The problem of reliability in computer modeling arises from the fact that CAE programs usually are not equipped with comprehensive material databases. We have solved this problem especially for casting simulation and molding materials, which can differ in composition at different plants and therefore cannot be combined into a common database. To determine unknown thermo-physical properties, the temperature had been measured in several points of solidifying cylindrical sample initially, and the appropriate computer simulation of the test technology was performed. Then the difference between the calculated and experimental temperatures was minimized using the modified Levenberg-Marquardt optimization algorithm.

1. Introduction

Simulation of technological processes intends to become an essential preproduction stage of digital manufacturing in machine building industry [1]. In particular, casting process simulation using CAE software is now widely accepted as an effective tool in product design and process development which allows to improve quality of cast machine parts [2]. There is a number of special programs for simulation of casting processes and predicting the technological defects inside the cast parts. Among the others, LVMFlow (known also as NovaFlow&Solid [3]) package is one of the most popular software tools for improving foundry operations. The common problem for all the mentioned programs is the lack of material properties suitable for modeling casting processes [4].

For the computation of non-stationary temperature fields and analysis of temperature-dependent processes such as solidification and melt flow, some principal parameters of numerical model have to be known, that are related to the coefficients of the heat conduction equations [5]. First of all, thermo-physical properties of alloys during solidification, specific heat capacity and the thermal conductivity, are critical data for successful work of the software solver [6]. Some properties have been measured for specific alloys with a relatively low melting point [7]. However, the number of alloys for which the necessary information is available is limited, primarily due to the difficulty in experimentally determining these properties at a high temperature process.

In addition to the properties of cast alloys, it is also necessary to know the exact properties of the molding materials [8]. Unfortunately, the properties of those materials are highly dependent on the specific processing and the composition, which can differ significantly at different foundries. In some cases, the temperature-dependent behavior of the molding materials is not considered in simulation because the required data are not available in the material database. The information may be incomplete in the material database because not all the properties have been measured. Sometimes, disparate information from a variety of sources is used to build up the database by customers. The latter situation can lead to inconsistent computation results.

Casting simulation requires high-quality information concerning thermo-physical and physical properties during solidification [9]. Some numerical optimization methods can be employed to calculate unknown values of material properties at high temperatures [10]. Levenberg-Marquardt method is one of the methods which allows to solve the inverse heat conduction problem, consider the differences between simulated and measured temperatures, and obtain the coefficients of the heat transfer equation needed for simulation of the casting process [11]. Being proposed for solving nonlinear equations, Levenberg-Marquardt method is widely used for solving inverse problems, which have a significant range of backgrounds in engineering applications [12].

To overcome the lack of data about directly measured thermo-physical properties of cast alloys and mold materials, it is highly desirable to develop computer models and computational methods for calculation of missing data. The main objective of this study is to develop an advanced method to identify temperature-dependent thermo-physical properties of cast alloys and mold making materials by solving an inverse heat conduction problem.

2. Numerical model for temperature computation

As the first step for investigating mold materials and expanding the material database with corrected properties, we have created the numerical model for temperature computation during solidification. The model was developed according to the requirements of simple geometry and possibility to verify the results of measuring temperatures by thermocouples during subsequent full-scale experiments. The numerical model created for simulations by preprocessor module of LVMFlow package allows to obtain temperature distribution for a cast alloy spaceman solidifying and cooling in a mold, which is made of unknown molding mixture.

All the materials of the model are considered to be isotropic and temperature-dependent. Two thermocouples are inserted into the 3D model at different locations of the casting in the horizontal plane of symmetry and include real components of platinum-rhodium thermocouples with appropriate material properties. Fig. 1a shows the meshed model and position of two virtual temperature sensors in the casting identical to the real thermocouples inside the mold, whereas distribution of simulated temperatures is illustrated in Fig. 1b.

In order to verify the numerical model, cylindrical specimens with diameter of 40 mm and length of 100 mm were solidified in the cylindrical sand mold. Thus, the analytical problem of calculating the three-dimensional temperature field is reduced to an axi-symmetric one. In the tests, the casting was poured with steel at 1590 ^{O}C and the temperature was recorded at two points of the casting by thermocouples. The composition of the cast steel follows the specifications of the standard (amount in wt %: C 0.2, Si 0.3 and the rest Fe); its thermo-physical properties needed for simulation are accurately measured and presented both in the literature [11] and in the material databases.

The mold initial temperature was at 25°C. The top surface of the mold and side of the mold exchange heat with the environment by free convection mode. The ambient temperature is taken as 25°C. The control volume mesh consisting of about 450 thousand cells was automatically generated according to the surfaces of the 3D model. The cooling time of about 1 hour was measured until the casting reaches the desired temperature of nearly 300 ^{O}C.

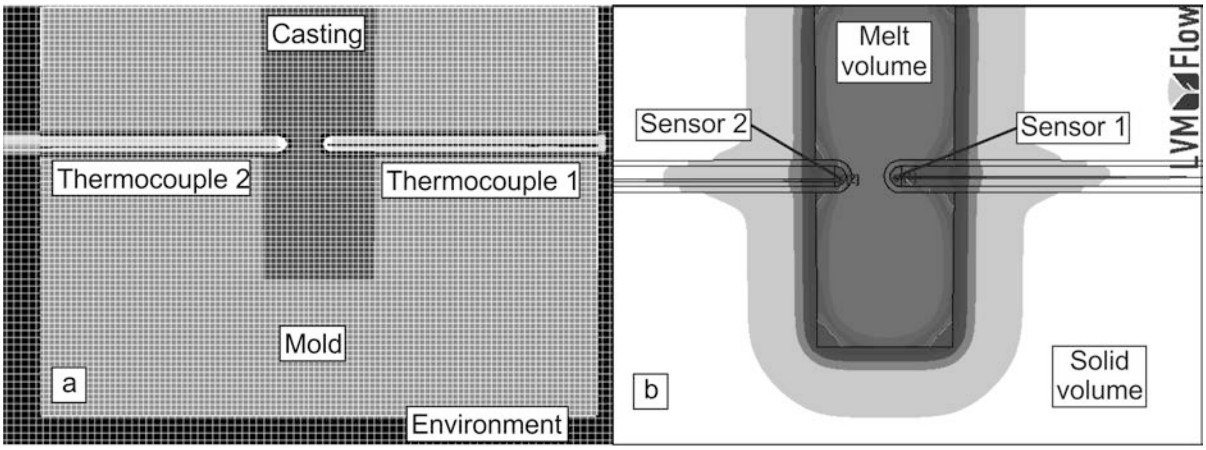

Figure 1. Temperature sensors in computational model (a) and distribution of simulated temperatures (b) in the vertical plane of symmetry.

The proposed method to simulate the temperature field in a casting and then make it identical to the experimentally observed data by correcting thermo-physical properties in the database can be applied not only to the considered cylindrical sample, but also to large-sized castings of complex shape. Accordingly, an experiment on measuring temperature with thermocouples at several points on the surface of the mold can be carried out in workshop conditions for real critical castings.

3. Optimization procedure

The prediction of possible technological defects in cast parts is based on the simulation of temperature fields by solving a nonlinear differential heat equation. The accuracy of solution highly depends on the coefficients included into the equation, which coefficients are the thermo-physical properties of materials, namely the specific heat capacity and the thermal conductivity.

In many cases, the thermo-physical properties required for simulation of foundry technology, especially their values at temperatures above the melting point of cast alloy, cannot be obtained by direct laboratory measurements for two reasons. Firstly, the composition of cast alloys or molding materials and the properties themselves may constitute a commercial secret. Secondly, solidification conditions for large castings in the workshop differ from the solidification conditions for a small sample in the laboratory. The latter is especially important for molding materials, since their properties, included into the database, could indirectly comprise not only heat transfer but also the boundary effects to ensure more accurate simulation. Moreover, the advantage of computational method of adjusting properties, in contrast to laboratory measurements, is the ability to investigate the short-living characteristics of the sand mold materials actually used in factory practice, which may contain water and degrading binders.

The basic idea of the optimization procedure in this work is to calculate the specific heat capacity and the thermal conductivity of the materials in the range from 20 to 1600 ^{O}C using some measured temperature values. For this purpose, the quality factor K is defined as a sum over all measured points $K = (\Sigma\, |T^M - T^S| \,/\, \Sigma\, T^S)$, where T^M and T^S are, respectively, measured and simulated temperatures.

The material properties are assembled to a vector $\mathbf{P}^k$. At each iteration step, the properties in the material database are changed and approached to the exact values in accordance with the quality factor $K \rightarrow 0$. The algorithm of the iterative solution can be represented in the form $\mathbf{P}^{k+1} = \mathbf{P}^k + \Delta P$, where ΔP is solution of the system of nonlinear equations $(J^T J - \mu J)\, \Delta P = -\, J^T \Delta T$ and J is the Jacobian matrix. Solving inverse problems is an optimization procedure of minimizing the objective function. The objective function in the Levenberg-Marquardt optimization is $S = \Sigma\, (T^M - T(P))^2$.

The advantage of the proposed optimization method can be revealed in the troublesome case when $|J^T J| \approx 0$, due to the use of the regularization parameter μ. When we assign large values to the μ

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parameter in the model, the applied optimization method becomes similar to the steepest descent method, whereas small μ values lead to iterations by the Gauss-Newton method.

The libraries of the MATLAB program and its computational capabilities for processing matrices were used to implement the proposed nonlinear optimization method. Using the MATLAB language, the program code for calculations was compiled and the necessary interface was created for data input and analysis.

4. Results of applying the optimization procedure

Computational experiments on modeling solidification of carbon steel for the test casting in a cylindrical mold were carried out using the LVMFlow software in accordance with full-scale experiment. The curves in Fig. 2a represent the registered temperature change in the cast alloy. Here the cooling curves obtained from the LVMFlow simulation results can be compared with the temperatures measured by thermocouple in the casting during its solidification process. The temperature curves at the considered points of the solidifying melt, shown in Fig. 2b, were found nearly identical in the simulation and experiment after the third iteration of improving the database set for the mold material.

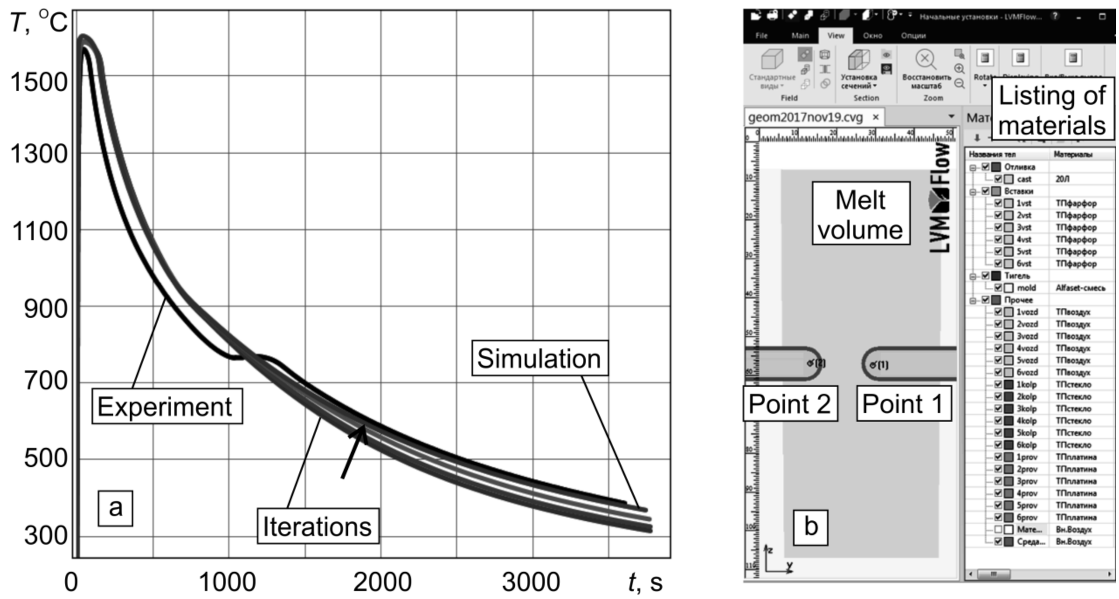

Figure 2. Temperature curves obtained in the simulation and corresponding experiment data (a) at the point 1 of thermocouple location (b)

5. Conclusion

In this research, the numerical model has been developed for simulation of casting and calculation of thermo-physical properties during solidification, that is suitable for improving database both of mold materials and cast alloys. This model was successfully combined with measuring temperature fields by thermocouples in laboratory for test casting and in foundry conditions for large castings. The Levenberg-Marquardt optimization method was adapted to determine specific heat capacity and thermal conductivity, so that the method has approximated the properties in three iterations of the model simulation by means of the CAE LVMFlow processor.

As a result, the properties can be determined for any CAE casting simulators to avoid the problem of incomplete databases and difficulties of their direct measuring in the high temperature interval. Further development of the proposed method is of great interest for simulation of cast alloys with special chemical compositions.

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